

Table 1: Wyckoff site: $1\mathbf{o}$, site symmetry: $6'22'$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]$

 Table 2: Wyckoff site: $2\mathbf{a}$, site symmetry: $6'..$

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 7, 8, 9]$
2	$[0, 0, -z]$	$[4, 5, 6, 10, 11, 12]$

 Table 3: Wyckoff site: $6\mathbf{b}$, site symmetry: $.2.$

No.	position	mapping
1	$[x, 0, 0]$	$[1, 4]$
2	$[0, x, 0]$	$[2, 5]$
3	$[-x, -x, 0]$	$[3, 6]$
4	$[-x, 0, 0]$	$[8, 11]$
5	$[0, -x, 0]$	$[9, 12]$
6	$[x, x, 0]$	$[7, 10]$

 Table 4: Wyckoff site: $6\mathbf{c}$, site symmetry: $..2$

No.	position	mapping
1	$[x, -x, 0]$	$[1, 12]$
2	$[x, 2x, 0]$	$[2, 10]$
3	$[-2x, -x, 0]$	$[3, 11]$
4	$[-x, x, 0]$	$[5, 8]$
5	$[-x, -2x, 0]$	$[6, 9]$
6	$[2x, x, 0]$	$[4, 7]$

 Table 5: Wyckoff site: $12\mathbf{d}$, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-y, x - y, z]$	$[2]$
3	$[-x + y, -x, z]$	$[3]$

continued ...

Table 5

No.	position	mapping
4	$[-x, -y, z]$	[8]
5	$[y, -x + y, z]$	[9]
6	$[x - y, x, z]$	[7]
7	$[y, x, -z]$	[5]
8	$[x - y, -y, -z]$	[4]
9	$[-x, -x + y, -z]$	[6]
10	$[-y, -x, -z]$	[12]
11	$[-x + y, y, -z]$	[11]
12	$[x, x - y, -z]$	[10]